Howard D. Flack*

Patterson functions

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Abstract: The paper deals with $|F|^2$, *A* and *D* Patterson functions. The information available in the various volumes of *International Tables for Crystallography* is detailed. *A* and *D* are defined and the reason for their use is explained. The symmetry of these functions is explained. Calculation by symmetry-adapted Patterson functions and the Fast-Fourier algorithm are described. There are two examples. There is a very useful table presenting the relevant information.

Keywords: International Tables for Crystallography; Patterson function; Patterson symmetry.

In memory of Hans Wondratschek

Introduction

Flack et al. [1] and Ackerbauer et al. [2] have made use of the *A*- and *D*-Patterson functions in novel applications for small-molecule crystallography. Amongst these it was found that these functions were powerful in detecting displaced or incorrectly assigned atoms and, especially in the case of the intermetallic compound TiGePt, of coming to a firm decision on whether the crystal structure was centrosymmetric or not. For the above two publications, the *A*- and *D*-Patterson functions were calculated by *ad-hoc* procedures. In the current publication, information is presented on the symmetry and methods of calculation of these Patterson functions, supplementing standard sources of material on this matter.

Although the *International Tables for Crystallography* contain a firm grounding of relevant information, it is spread amongst the three volumes A [3], B [4, 5] and C [6] with the further disadvantage that the relevance to the Patterson functions of some tables of values is not clearly stated or explained. The necessity of a short combined compilation of values was evident. This is given in Table 1 with the theory presented briefly as text.

***Corresponding author: Howard D. Flack,** Chimie minérale, analytique et appliquée, University of Geneva, Switzerland, E-mail: crystal@flack.ch

A and *D*

In the works of Flack et al. [1], Parsons et al. [7] and Ackerbauer et al. [2], it was found that the *A*- and *D*-Patterson functions were more useful and gave clearer results than the $|F|^2$ Patterson. *A* and *D* are defined as the average (*A*) and difference (*D*) of Friedel opposites (*hkl* and $\bar{h}\,\bar{k}\,\bar{l}$):

$$A(hkl) = \tfrac{1}{2}[|F(hkl)|^2 + |F(\bar{h}\,\bar{k}\,\bar{l})|^2], \tag{1a}$$

$$D(hkl) = |F(hkl)|^2 - |F(\bar{h}\,\bar{k}\,\bar{l})|^2. \tag{1b}$$

In the spherical atom approximation without atomic displacement parameters, $A(hkl)$ and $D(hkl)$ may be expressed as follows:

$$A(hkl) = \sum_m \sum_n [(f_m + f'_m)(f_n + f'_n) + f''_m f''_n] \cdot \cos\{2\pi[h(x_m - x_n) + k(y_m - y_n) + l(z_m - z_n)]\}, \tag{2a}$$

$$D(hkl) = \sum_m \sum_n [(f_m + f'_m) f''_n - (f_n + f'_n) f''_m] \cdot \sin\{2\pi[h(x_m - x_n) + k(y_m - y_n) + l(z_m - z_n)]\}, \tag{2b}$$

where f_m is the free atom scattering factor of atom m, f'_m and f''_m are its real and imaginary components of the resonant scattering factor, and x_m, y_m, z_m are the fractional coordinates of atom m.

The inverse Fourier transforms of the $A(hkl)$ and the $D(hkl)$ are the real Patterson functions $P_A(uvw)$ and $P_D(uvw)$:

$$P_A(uvw) = \sum A(hkl) \cos[2\pi(hu + kv + lw)], \tag{3a}$$

$$P_D(uvw) = \sum D(hkl) \sin[2\pi(hu + kv + lw)], \tag{3b}$$

whilst the inverse Fourier transform of the $|F(hkl)|^2$ is the complex Patterson function $P_{|F|^2}(uvw)$:

$$P_{|F|^2}(uvw) = \sum |F(hkl)|^2 \{\cos[2\pi(hu + kv + lw)] + i\sin[2\pi(hu + kv + lw)]\}. \tag{4}$$

When making use of the A and the D, the intensity data must first be separated into three classes: (p) pairs of Friedel opposites of acentric reflections, (u) unpaired acentric reflections and (c) centric reflections. This classification is dependent on the point group of the crystal structure and relevant values are presented in Table 1 of Shmueli and Flack [8].

Tab. 1: Patterson symmetries and symmetries of Patterson functions for space groups.[1]

Space-group types		Patterson
H-M symbols	**Nos.**	**Symmetry**
Crystal family triclinic (anorthic), Bravais-lattice type *aP*		
***P*1**	**1**	$P\bar{1}$
***P*$\bar{1}$**	**2**	$P\bar{1}$
Crystal family monoclinic, Bravais-lattice type *mP*		
***P*2**–$P2_1$	**3**–4	$P2/m$
Pm–Pc	**6**–7	$P2/m$
P*2/*m–$P2_1/m$,	**10**–11	$P2/m$
$P2/c$–$P2_1/c$	13–14	$P2/m$
Crystal family monoclinic, Bravais-lattice type *mS*		
***C*2**	**5**	$C2/m$
Cm–Cc	**8**–9	$C2/m$
C*2/*m, $C2/c$	**12**, 15	$C2/m$
Crystal family orthorhombic, Bravais-lattice type *oP*		
***P*222**–$P2_12_12_1$	**16**–19	$Pmmm$
***Pmm*2**–$Pnn2$	**25**–34	$Pmmm$
Pmmm–$Pnma$	**47**–62	$Pmmm$
Crystal family orthorhombic, Bravais-lattice type *oS*		
$C222_1$, ***C*222**	20, **21**	$Cmmm$
***Cmm*2**–$Ccc2$	**35**–37	$Cmmm$
***Amm*2**–$Aea2$	**38**–41	$Ammm$
$Cmcm$–$Cmce$, ***Cmmm***,	63–64, **65**	$Cmmm$
$Cccm$–$Ccce$	66–68	$Cmmm$
Crystal family orthorhombic, Bravais-lattice type *oF*		
***F*222**	**22**	$Fmmm$
***Fmm*2**–$Fdd2$	**42**–43	$Fmmm$
Fmmm–$Fddd$	**69**–70	$Fmmm$
Crystal family orthorhombic, Bravais-lattice type *oI*		
***I*222**–$I2_12_12_1$	**23**–24	$Immm$
***Imm*2**–$Ima2$	**44**–46	$Immm$
Immm–$Imma$	**71**–74	$Immm$
Crystal family tetragonal, Bravais-lattice type *tP*		
***P*4**–$P4_3$	**75**–78	$P4/m$
***P*$\bar{4}$**	**81**	$P4/m$
P*4/*m–$P4_2/n$	**83**–86	$P4/m$
***P*422**–$P4_32_12$	**89**–96	$P4/mmm$
P*4*mm–$P4_2bc$	**99**–106	$P4/mmm$
P*$\bar{4}$2*m–$P\bar{4}2_1c$	**111**–114	$P4/mmm$
***P*$\bar{4}$*m*2**–$P\bar{4}n2$	**115**–118	$P4/mmm$
P*4/*mmm–$P4_2/ncm$	**123**–138	$P4/mmm$

Tab. 1 (continued)

Space-group types		Patterson
H-M symbols	**Nos.**	**Symmetry**
Crystal family tetragonal, Bravais-lattice type *tI*		
***I*4**, $I4_1$	**79**–80	$I4/m$
***I*$\bar{4}$**	**82**	$I4/m$
I*4/*m–$I4_1/a$	**87**–88	$I4/m$
***I*422**–$I4_122$	**97**–98	$I4/mmm$
I*4*mm–$I4_1cd$	**107**–110	$I4/mmm$
***I*$\bar{4}$*m*2**–$I\bar{4}c2$	**119**–120	$I4/mmm$
***I*$\bar{4}$2m**–$I\bar{4}2d$	**121**–122	$I4/mmm$
I*4/*mmm–$I4_1/acd$	**139**–142	$I4/mmm$
Crystal family hexagonal, Bravais-lattice type *hP*		
***P*3**–$P3_2$	**143**–145	$P\bar{3}$
***P*$\bar{3}$**	**147**	$P\bar{3}$
***P*312**, $P3_112$, $P3_212$	**149**, 151, 153	$P\bar{3}1m$
***P*321**, $P3_121$, $P3_221$	**150**, 152, 154	$P\bar{3}m1$
***P*3*m*1**, $P3c1$	**156**, 158	$P\bar{3}m1$
P*31*m, $P31c$	**157**, 159	$P\bar{3}1m$
P*$\bar{3}$1*m–$P\bar{3}1c$	**162**–163	$P\bar{3}1m$
***P*$\bar{3}$*m*1**–$P\bar{3}c1$	**164**–165	$P\bar{3}m1$
***P*6**–$P6_3$	**168**–173	$P6/m$
***P*$\bar{6}$**	**174**	$P6/m$
P*6/*m–$P6_3/m$	**175**–176	$P6/m$
***P*622**–$P6_322$	**177**–182	$P6/mmm$
P*6*mm–$P6_3mc$	**183**–186	$P6/mmm$
***P*$\bar{6}$*m*2**–$P\bar{6}c2$	**187**–188	$P6/mmm$
P*$\bar{6}$2*m–$P\bar{6}2c$	**189**–190	$P6/mmm$
P*6/*mmm–$P6_3/mmc$	**191**–194	$P6/mmm$
Crystal family hexagonal, Bravais-lattice type *hR*		
***R*3**	**146**	$R\bar{3}$
***R*$\bar{3}$**	**148**	$R\bar{3}$
***R*32**	**155**	$R\bar{3}m$
R*3*m–$R3c$	**160**–161	$R\bar{3}m$
R*$\bar{3}$*m–$R\bar{3}c$	**166**–167	$R\bar{3}m$
Crystal family cubic, Bravais-lattice type *cP*		
***P*23**, $P2_13$	**195**, 198	$Pm\bar{3}$
***Pm*$\bar{3}$**–$Pn\bar{3}$, $Pa\bar{3}$	**200**–201, 205	$Pm\bar{3}$
***P*432**–$P4_232$,	**207**–208,	$Pm\bar{3}m$
$P4_332$–$P4_132$	212–213	$Pm\bar{3}m$
P*$\bar{4}$3*m, $P\bar{4}3n$	**215**, 218	$Pm\bar{3}m$
Pm*$\bar{3}$*m–$Pn\bar{3}m$	**221**–224	$Pm\bar{3}m$
Crystal family cubic, Bravais-lattice type *cF*		
***F*23**	**196**	$Fm\bar{3}$
***Fm*$\bar{3}$**–$Fd\bar{3}$	**202**–203	$Fm\bar{3}$
***F*432**–$F4_132$	**209**–210	$Fm\bar{3}m$
F*$\bar{4}$3*m–$F\bar{4}3c$	**216**, 219	$Fm\bar{3}m$
Fm*$\bar{3}$*m–$Fd\bar{3}c$	**225**–228	$Fm\bar{3}m$
Crystal family cubic, Bravais-lattice type *cI*		
***I*23**, $I2_13$	**197**, 199	$Im\bar{3}$
***Im*$\bar{3}$**, $Ia\bar{3}$	**204**, 206	$Im\bar{3}$
***I*432**, $I4_132$	**211**, 214	$Im\bar{3}m$
I*$\bar{4}$3*m, $I\bar{4}3d$	**217**, 220	$Im\bar{3}m$
Im*$\bar{3}$*m–$Ia\bar{3}d$	**229**–230	$Im\bar{3}m$

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[1]The space-group types of each row form an arithmetic crystal class. (In three instances the row is typeset on two lines.) The arithmetic crystal class is identified by its representative symmorphic space group for which both the H-M symbol and the space-group type number are typeset in bold. A set of space groups with sequential numbers is indicated by the symbols of the first and last space group of the sequence separated by a hyphen.

The column entitled *Patterson symmetry* indicates the symmetry of the set of interatomic vectors of crystal structures described in the space groups given in the column *Space-group types*. The *Patterson symmetry* is also the symmetry of the *A*-Patterson function, and the real part of the complex $|F|^2$-Patterson.

The crystallographic symmetry of both the *D*-Patterson function and the imaginary part of the complex $|F|^2$ Patterson is that of the symmorphic space group of crystal structures described in the space groups given in the column *Space-group types*. To this crystallographic symmetry, the non-crystallographic operation of a centre of anti-symmetry needs to be added to give $P_D(uvw) = -P_D(\bar{u}\,\bar{v}\,\bar{w})$.

The setting and origin choice of the chosen space group should also be used for the space group of the Patterson symmetry and the symmorphic space group.

International Tables for Crystallography

Reference is made here to the relevant sections of International Tables for Crystallography, Volumes A [3], B [4, 5] and C [6].

In Volume A, [9], one finds the value *Patterson symmetry* given in the heading of each of the 230 space groups. This value gives the symmetry of the 'vector set' generated by the operation of the space group on an arbitrary set of general positions. It may also be described as the symmetry of the set of the interatomic vectors of a crystal structure with the selected space group. The Patterson symmetry is a crystallographic space group denoted by its Hermann-Mauguin symbol. It is in fact one of the 24 centrosymmetric symmorphic space groups which have been taken as representatives of the corresponding arithmetic classes. Most unfortunately the content in Volume A, [3] on arithmetic crystal classes is incomplete, see Wilson [10]. These are mentioned by Wondratschek [11]. There is no table of values indicating those space groups belonging to each arithmetic crystal class nor the symmorphic space groups chosen as representatives of each class.

In Volume B, Bricogne [12] presents the theoretical basis of the Patterson function and the Harker vectors. There is an excellent chapter on the Patterson function by Tong et al. [13], especially in its applications to macromolecular compounds. Algorithms for the numerical evaluation of the Patterson function are not presented. Shmueli [4, 5] presents the space-group adapted trigonometric expressions of structure factors for all the space groups but does not mention how these may be used in the evaluation of a Patterson function. Reference should be made to the section *Symmetry-adapted Patterson functions* and *Example 2* of the current publication for relevant information. Finally, Millane [14] apply cylindrically-averaged Patterson functions in X-ray fibre diffraction analysis.

In Volume C, Wilson [10] presents useful tables of values and text concerning the arithmetic crystal classes. However Wilson's compilation neither indicates the Bravais-lattice type, nor the symmorphic space group representative of each arithmetic class nor the centrosymmetric supergroup of lowest index of the latter for each space group. However Wilson [10, 15] does give information on the symmetry of the $|F|^2$ Patterson function by stating: *… the symmetry of the Patterson synthesis … will be that of the symmorphic space group belonging to the arithmetic crystal class to which the space group of the structure belongs. An equivalent description of such symmetries, in terms of 73 of the 1651 dichromatic colour groups, has been given by* Fischer and Knof [16]. Wilson [17] has given further consideration to the apparent incompatibility in the definition of the symmetry of the $|F|^2$ Patterson function as used by No-author [9] and Fischer and Knof [16]. The practical application of this analysis is limited and will not be used in the current paper. No-author [9] does not indicate the symmetry of the $|F|^2$ Patterson function as stated by Wilson [10] and Fischer and Knof [16].

Symmetry

Concerning the symmetry of the P_A and P_D functions, we may use the statement of Wilson [10, 15], quoted above, as a starting point. All three Patterson functions (i.e. on $|F|^2$, *A* and *D*) possess the symmetry of the symmorphic space group representative of the arithmetic crystal class to which the space group belongs. However the linear combinations of $|F(hkl)|^2$ and $|F(\bar{h}\,\bar{k}\,\bar{l})|^2$ used to define $A(hkl)$ and $D(hkl)$ introduce further symmetry.

By definition $A(hkl) = A(\bar{h}\,\bar{k}\,\bar{l})$ and consequently $P_A(uvw) = P_A(\bar{u}\bar{v}\bar{w})$. It follows that P_A displays the symmetry of the centrosymmetric supergroup of lowest index of the symmorphic space group representative of the arithmetic crystal class to which the space group of the crystal

structure belongs. If the space group is centrosymmetric, then it is the symmorphic space group itself which has to be used. The entry *Patterson symmetry* of No-author [9] is the full symmetry of the *A*-Patterson function whether the space group is centrosymmetric or not, and whether resonant scattering is significant or not. As already stated above, the *Patterson symmetry* is in all cases the symmetry of the set of interatomic vectors.

By definition $D(hkl) = -D(\bar{h}\,\bar{k}\,\bar{l})$ and consequently $P_D(uvw)$ is antisymmetric with $P_D(uvw) = -P_D(\bar{u}\,\bar{v}\,\bar{w})$. This latter relation is not that of any crystallographic symmetry operation, so the full expression of the symmetry of $P_D(uvw)$ is not that of any space group. $P_D(uvw)$ displays the symmetry of the symmorphic space group representative of the arithmetic crystal class to which the space group of the crystal structure belongs. To this crystallographic symmetry is added that of a centre of antisymmetry, $P_D(uvw) = -P_D(\bar{u}\,\bar{v}\,\bar{w})$. The symmetry of $P_D(uvw)$ is not displayed by No-author [9].

The complex Patterson function on $|F|^2$ may use reflections from all three classes p, u and c defined above. However for $P_A(uvw)$ one uses only reflections from the two classes p and c, whereas for $P_D(uvw)$ only reflections from class p are appropriate. It may also be satisfactory to use the value $|F(hkl)|^2$ of an unpaired acentric reflection, both as reflection *hkl* and as reflection $\bar{h}\,\bar{k}\,\bar{l}$ with identical values of $|F(hkl)|^2$, as the value of $A(hkl)$ in the calculation of $P_A(uvw)$. The corresponding value of $D(hkl)$ is zero. The multiplicity of reflections as used in $|F|^2$, *A* and *D* Patterson syntheses are identical.

The asymmetric units of $P_{|F|^2}(uvw)$, $P_A(uvw)$ and $P_D(uvw)$ are identical, being those of the symmorphic space group. The values of $A_{\text{model}}(000)$ and $D_{\text{model}}(000)$ are given by $A_{\text{model}}(000) = \Sigma\Sigma\,[(f_m + f'_m)(f_n + f'_n) + f''_m f''_n]$ and $D_{\text{model}}(000) = 0$. The corresponding observed values can not be measured.

Evaluation of Patterson functions

It is of practical value in certain circumstances to have the trigonometric expressions for the P_A and P_D functions adapted to the known (or presumed) space group of the crystal structure. These expressions are given for all 230 space groups by Shmueli [4, 5]. One proceeds as follows. From the space group, one first identifies its arithmetic crystal class. Next one identifies the symmorphic space group representative of the arithmetic crystal class. Then in tables 1.4 of Shmueli [4, 5], one uses the entry for this symmorphic space group. The trigonometric expression in the column marked "A" of this symmorphic space group is the one valid for $P_A(uvw)$. That in the column marked "B" is that of $P_D(uvw)$. Relevant values for locating the expression are displayed in Table 1.

The Cooley and Tukey [18] algorithm of fast-Fourier transform (FFT) may also be used in the evaluation of the *A*- and *D*-Patterson functions. One proceeds by writing the general complex Fourier transform of $|F|^2$ in space group *P*1 as given in equation (4) as:

$$P_{|F|^2}(uvw) = 1/V \sum(\text{whole sphere})\,|F(hkl)|^2 \exp[-2\pi i(hu + kv + lw)], \quad (5)$$

and then collecting together terms in Friedel opposites, *hkl* and $\bar{h}\,\bar{k}\,\bar{l}$ to obtain

$$P_{|F|^2}(uvw) = 2/V \sum(\text{hemisphere})\,A(hkl) \cos[2\pi(hu + kv + lw)] - i/V \sum(\text{hemisphere}) D(hkl) \sin[2\pi(hu + kv + lw)] = P_A(uvw) - iP_D(uvw). \quad (6)$$

One sees that the complex Fourier transform of $|F(hkl)|^2$, $P_{|F|^2}(uvw)$, calculated according to equation (5), gives $P_A(uvw)$ as its real part and $P_D(uvw)$ as its imaginary part under the following conditions:

(a) centric reflections are included in the sum of equation (5) both as reflection *hkl* and as reflection $\bar{h}\,\bar{k}\,\bar{l}$ with identical values of $|F(hkl)|^2$,
(b) unpaired acentric reflections are excluded from the sum in equation (5). It may also be satisfactory to use the value $|F(hkl)|^2$ of an unpaired acentric reflection both as reflection *hkl* and as reflection $\bar{h}\,\bar{k}\,\bar{l}$ with identical values of $|F(hkl)|^2$.

The inclusion of crystallographic symmetry in the FFT algorithm has been treated in many publications, see, for example, Ten Eyck [19], Bantz and Zwick [20], Immirzi [21], Auslander et al. [22] and Langs [23]. The appropriate crystallographic symmetry is that of the symmorphic space group of the crystal's space group given in Table 1.

Interpretation of Patterson functions

As shown in equation (3), the inverse Fourier transforms of the $A(hkl)$ and the $D(hkl)$ are the Patterson functions

$P_A(uvw)$ and $P_D(uvw)$. From equation 2, it is clear that these show peaks at the positions of the interatomic vectors $x_m - x_n$, $y_m - y_n$, $z_m - z_n$. The heights of the peaks are determined by the values of the pre-trigonometric factors in equation (2).

For $P_A(uvw)$, in general, the pre-trigonometric factor $(f_m + f'_m)(f_n + f'_n) + f''_m f''_n$ is always positive and approximately equal to $Z_m Z_n$, where Z_m is the number of electrons in atom or ion m. As a consequence, all interatomic vectors contribute and there is a large number of peaks in $P_A(uvw)$, resulting in a considerable amount of overlap. There is also a very large peak at the origin of $P_A(uvw)$. It follows that the interpretation of $P_A(uvw)$ in terms of atomic positions is difficult for structures with many atoms in the unit cell.

For $P_D(uvw)$, the pre-trigonometric factor $(f_m + f'_m) f''_n - (f_n + f'_n) f''_m$ may be positive, zero or negative. In general the magnitude of this factor is small due to the small magnitude of the values of the f''_m. Moreover, this pre-trigonometric factor is zero if atoms m and n are of the same chemical element. The weakness of $|D(hkl)|$ has two causes: the small values of $|f''_m|$ and the limited number of contributing interatomic vectors. As a considerable number of interatomic vectors do not contribute, $P_D(uvw)$ suffers much less from overlap and may be easier to interpret than $P_A(uvw)$. There is no origin peak in $P_D(uvw)$. The $D(hkl)$ and $P_D(uvw)$ are zero for a centrosymmetric structure.

It is necessary to be aware that there is an experimental limitation in the use of $P_D(uvw)$. The problem arises because the values of D_{obs} are frequently dominated by random uncertainties and systematic errors which swamp out the resonant-scattering signal. Experience shows that in ~33% data sets, the resonant scattering signal is clearly observed, whereas in another ~33%, this signal has been lost. The remaining ~33% data sets are intermediate. Although in light-atom compounds the resonant-scattering is necessarily small, it may nevertheless be observable. It is quite possible not to observe the resonant-scattering signal in heavy-atom compounds. Peaks in $|P_D(uvw)|$ should occur at the same position as a large value of $P_A(uvw)$ to be of structural significance since both arise at the positions of interatomic vectors. Indeed this property could be used as a data-evaluation technique prior to structure solution.

The use of Harker lines and sections in the interpretation of Patterson functions applies both to $P_A(uvw)$ and $P_D(uvw)$.

Examples

Example 1

A crystal structure is assumed to be in the space group $P2_12_12_1$. This has space-group type number 19 and from Table 1 is seen to have Bravais-lattice type *oP* in the orthorhombic family. The geometric class is 222 and the arithmetic class is 222*P* with symmorphic space group *P*222, space-group type number 16. The symmetry of the *A*-Patterson function is *Pmmm* and that of the *D*-Patterson function is *P*222 additionally with the antisymmetry $P_D(uvw) = -P_D(\bar{u}\bar{v}\bar{w})$. For the calculation of the *A*-Patterson one uses both the values of $|F|^2$ of the centric reflections (0*kl*, *h*0*l*, *hk*0) [see table 1 of Shmueli and Flack [8]] and *A* of the paired acentric reflections (*hkl*, $\bar{h}\bar{k}\bar{l}$). For the calculation of the *D*-Patterson one uses only the values of *D* of the paired acentric reflections (*hkl*, $\bar{h}\bar{k}\bar{l}$). For the form of the symmetry-adapted Patterson function, one uses the entry for the symmorphic space group *P*222, space-group type number 16 from Shmueli [4, 5]. One finds for the *A*-Patterson function the term 4ccc [i.e. $4\cos(2\pi hu)\cos(2\pi kv)\cos(2\pi lw)$] and for the *D*-Patterson function −4sss [i.e. $-4\sin(2\pi hu)\sin(2\pi kv)\cos(2\pi lw)$].

Example 2

A crystal structure is assumed to be in the space group *R*32 and hexagonal axes in the obverse setting have been used. The space-group type number is 155 and from Table 1 is seen to have Bravais-lattice type *hR* in the hexagonal family. The geometric class is 32 and the arithmetic class is 32*R* with symmorphic space group *R*32, space-group type number 155. The symmetry of the *A*-Patterson function is $R\bar{3}m$ and that of the *D*-Patterson function is *R*32 additionally with the antisymmetry $P_D(uvw) = -P_D(\bar{u}\bar{v}\bar{w})$. For the calculation of the *A*-Patterson one uses both the values of $|F|^2$ of the centric reflections (*h*0*l*) [see table 1 of Shmueli and Flack [8]] and *A* of the paired acentric reflections (*hkl*, $\bar{h}\bar{k}\bar{l}$; *hh*0, $\bar{h}\bar{h}$0). For the calculation of the *D*-Patterson one uses only the values of *D* of the paired acentric reflections (*hkl*, $\bar{h}\bar{k}\bar{l}$; *hh*0, $\bar{h}\bar{h}$0). For the form of the symmetry-adapted Patterson function, one uses the entry for the symmorphic space group *R*32, space-group type number 155 from Shmueli [4, 5]. One finds for the *A*-Patterson function the term 3[PH(cc)c(*lz*) − MH(ss)s(*lz*)] i.e. $3(\{\cos[2\pi(hu + kv)] + \cos[2\pi(ku + iv)] + \cos[2\pi(iu + hv)] + \cos[2\pi(ku + hv)] + \cos[2\pi(hu + iv)] + \cos[2\pi(iu + kv)]\}\cos(2\pi lw) - \{\sin[2\pi(hu + kv)] + \sin[2\pi(ku + iv)] + \sin[2\pi(iu + hv)] - \sin$

$[2\pi(ku + hv)] - \sin[2\pi(hu + iv)] - \sin[2\pi(iu + kv)]\}\sin(2\pi lw))$ and for the *D*-Patterson function $3[\mathrm{PH(ss)c}(lz) + \mathrm{MH(cc)s}(lz)]$ i.e. $3(\{\sin[2\pi(hu + kv)] + \sin[2\pi(ku + iv)] + \sin[2\pi(iu + hv)] + \sin[2\pi(ku + hv)] + \sin[2\pi(hu + iv)] + \sin[2\pi(iu + kv)]\}\cos(2\pi lw) + \{\cos[2\pi(hu + kv)] + \cos[2\pi(ku + iv)] + \cos[2\pi(iu + hv)] - \cos[2\pi(ku + hv)] - \cos[2\pi(hu + iv)] - \cos[2\pi(iu + kv)]\}\sin(2\pi lw))$.

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